THE CHALLENGE FOR MATERIALS DESIGN

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The dependence of material behavior, as measured by properties and performance, on structure and processing forms the principal axiom of materials science and engineering. The application of this fundamental truth to the rational design of materials for specific applications has emerged as one of the most challenging technical problems currently facing our industrial society. It is now generally recognized that this is the principal limiting factor in the application of new materials to engineering components. The typical design process begins with specifying a set of functional requirements for a component, followed by the optimization of a product design that uses a set of material properties obtained from a database. In the last twenty years the use of simulation and modeling in the computational part of the design process has reduced the product cycle from years to months by reducing the need for costly prototyping and serial experimentation. However, the materials database remains essentially unchanged due to the absence of similar advances in the design of materials. The development of new materials and processes remains a largely empirical endeavor guided largely by intuition with little quantitative scientific input.

Future advances in the reduction of product cycle time, agility of the manufacturing process and the development of optimal materials for engineering applications depends on advances in our ability to generate reliable quantitative models of materials and processes that can be coupled with design codes. This calls for the development of interoperable multiscale models of materials ranging from *ab initio* to continuum models. While increases in computing power will aid this process, the most important developments will come in the development of interoperable, physics-based models of material structure and properties at various length and time scales in forms that permit computation to reduce the lengthy experimentation currently required to produce reliable material data bases. This is the challenge to the next generation of mechanists and materials scientists and engineers.

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